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Relationship between vanishing splitting errors and pairwise commutativity

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Abstract

It has been shown that the commutativity of the two sub-operators in different operator splitting discretizations implies zero splitting error. This work investigates whether this commutativity condition is necessary for zero splitting error for some given operator splittings. The case of more than two sub-operators is also discussed, but there are still some open problems (see the end of this work).

Keywords: Operator splitting; Local splitting error; Commutativity conditions; Commutator; Time discretization

1. Introduction

In this work we consider the Cauchy problem

$$\frac{\mathrm{d}u(t)}{\mathrm{d}t} = Au(t), \quad t \in (0, T], \quad u(0) = u_0 \tag{1.1}$$

where X is a Banach space, $u : [0, T] \to X$ is the unknown function, A is a bounded linear operator $X \to X$, and $u_0 \in X$ a given initial function. Later on we denote the problem (1.1) by CP$(A, u_0, [0, T])$, whose solution is clearly $u(t) = \exp(At)u_0$. We assume that $A = \sum_{i=1}^{m} A_i$, where usually the sub-operators A_i have simpler structure than A. (This means that the problems CP$(A_i, u_0, [0, T])$ can be solved more efficiently than CP$(A, u_0, [0, T])$.)
Operator splitting is a time discretization method which exploits the above special structure of the operator A. In Section 2 we introduce the basics of this method and define the algorithms of some widely used concrete schemes. In Section 3 we analyze the accuracy of these splitting schemes, focusing on the question of whether the commutativity of each pair of sub-operators is necessary for zero splitting error.

2. The operator splitting method

Let us consider the Cauchy problem (1.1) and we define the mesh $\omega_\tau := \{t_n, n = 1, 2, \ldots N, N\tau = T\}$, where $\tau \ll T$ denotes the splitting time step. (For simplicity, we consider a uniform mesh.) Operator splitting is

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a time discretization technique, which defines an approximation to the solution of problem CP(A, u_0, $[0, T]$) at the mesh-points t_n. This method is based on replacing (1.1) with an appropriately defined sequence of Cauchy problems CP(A_i, u_{initial}, $[t_*, t^*]$), where t_* and t^* are mesh-points.
The algorithms of the most popular splitting methods are the following. (The notation $u_i(t)$ stands for the solution of CP(A_i, u_{initial}, $[t_*, t^*]$).)

- *Sequential splitting*. At each sub-interval $[t_n, t_{n+1}]$ we solve the problems with operators A_i, $i = 1, 2, \ldots, m$, successively, while each sub-problem uses the solution of the previous sub-problem as an initial condition. Algorithmically:

$$\begin{aligned}
&u_{\text{sp}}(0) = u_0\\
&\textbf{for } n = 0, N-1 \ (1)\\
&\quad u_0(t_{n+1}) = u_{\text{sp}}(t_n)\\
&\quad\quad \textbf{for } i = 1, m \ (1)\\
&\quad\quad\quad \text{CP}(A_i, u_{i-1}(t_{n+1}), [t_n, t_{n+1}])\\
&\quad\quad \textbf{end}\\
&\quad u_{\text{sp}}(t_{n+1}) = u_m(t_{n+1})\\
&\textbf{end}
\end{aligned} \tag{2.2}$$

- *Symmetric splittings*. At each time step we first solve the problems with operators A_i, $i = 1, 2, \ldots, m-1$, successively over the interval $[t_n, t_n + \tau/2]$, then apply operator A_m on the whole interval $[t_n, t_{n+1}]$, and finally, on $[t_n + \tau/2, t_{n+1}]$ the operators A_i, $i = m-1, m-2, \ldots, 1$, are applied. Again each sub-problem uses the solution of the previously solved sub-problem as an initial condition. This procedure can be given by the following algorithm:

$$\begin{aligned}
&u_{\text{sp}}(0) = u_0\\
&\textbf{for } n = 0, N-1 \ (1)\\
&\quad u_0(t_{n+0.5}) = u_{\text{sp}}(t_n)\\
&\quad\quad \textbf{for } i = 1, m-1 \ (1)\\
&\quad\quad\quad \text{CP}(A_i, u_{i-1}(t_{n+0.5}), [t_n, t_{n+0.5}])\\
&\quad\quad \textbf{end}\\
&\quad\quad\quad \text{CP}(A_m, u_{m-1}(t_{n+0.5}), [t_n, t_{n+1}])\\
&\quad\quad \textbf{for } i = m-1, 1 \ (-1)\\
&\quad\quad\quad \text{CP}(A_i, u_{i+1}(t_{n+1}), [t_{n+0.5}, t_{n+1}])\\
&\quad\quad \textbf{end}\\
&\quad u_{\text{sp}}(t_{n+1}) = u_1(t_{n+1})\\
&\textbf{end}
\end{aligned} \tag{2.3}$$

  where $t_{n+0.5} = (n + 0.5)\tau$ additional mesh-points. The scheme belonging to $m = 2$ is called Marchuk–Strang (MS) splitting [4,6].
- *Symmetrically weighted sequential (SWS) splitting*. At each splitting time step we average symmetrically the results of two sequential splittings, performed in reverse orders of the sub-operators, as the following algorithm shows:

$$\begin{aligned}
&u_{\text{sp}}(0) = u_0\\
&\textbf{for } n = 0, N-1 \ (1)\\
&\quad u_0^{(1)}(t_{n+1}) = u_0^{(2)}(t_{n+1}) = u_{\text{sp}}(t_n)\\
&\quad\quad \textbf{for } i = 1, m \ (1)\\
&\quad\quad\quad \text{CP}(A_i, u_{i-1}^{(1)}(t_{n+1}), [t_n, t_{n+1}])\\
&\quad\quad \textbf{end}\\
&\quad\quad \textbf{for } i = m, 1 \ (-1)\\
&\quad\quad\quad \text{CP}(A_i, u_{m-i}^{(2)}(t_{n+1}), [t_n, t_{n+1}])\\
&\quad\quad \textbf{end}\\
&\quad u_{\text{sp}}(t_{n+1}) = 0.5(u_m^{(1)}(t_{n+1}) + u_m^{(2)}(t_{n+1}))\\
&\textbf{end}
\end{aligned} \tag{2.4}$$

The general scheme of the operator splitting discretization can be given in the form of the one-step recursion

$$\left.\begin{array}{c} u_{\mathrm{sp}}(t_{n+1}) = S(\tau)u_{\mathrm{sp}}(t_n) \\ u_{\mathrm{sp}}(0) = u_0 \end{array}\right\} \tag{2.5}$$

for $n = 1, 2 \ldots, N$, where $S(\tau)$ is defined by the applied splitting method. For the above cases it has the form

- $S_{\mathrm{seq}}(\tau) = \mathrm{e}^{A_2\tau}\mathrm{e}^{A_1\tau}$;
- $S_{\mathrm{MS}}(\tau) = \mathrm{e}^{\frac{A_1}{2}\tau}\mathrm{e}^{A_2\tau}\mathrm{e}^{\frac{A_1}{2}\tau}$;
- $S_{\mathrm{SWS}}(\tau) = 0.5(\mathrm{e}^{A_2\tau}\mathrm{e}^{A_1\tau} + \mathrm{e}^{A_1\tau}\mathrm{e}^{A_2\tau})$.

3. The local splitting error and its disappearance

In general, the use of an operator splitting method, even if each sub-problem is solved exactly, results in the appearance of the so-called local splitting error, which is defined as

$$\mathrm{Err}_{\mathrm{sp}}(\tau) = u(\tau) - u_{\mathrm{sp}}(\tau). \tag{3.6}$$

Since this error coincides with the local error of the operator splitting method as a time discretization scheme, we require the relation $\mathrm{Err}_{\mathrm{sp}}(\tau) = \mathcal{O}(\tau^{p+1})$ by some $p > 0$. The number p is called the order of the splitting method. As an easy computation shows, the sequential splitting is a first-order splitting method, while the MS splitting and the SWS splitting are second-order splitting methods [5,1,3]. In the case of stability of the splittings, higher local error order implies faster convergence of the splitting solution to the exact solution as the splitting time step tends to zero. The issue of stability is not considered here. We only remark that there are some special cases where the stability of a splitting method follows easily. For example, this is trivially the case if the sub-operators define contractive problems. Otherwise further investigations are necessary.

Obviously, it would be desirable that the local splitting error vanish. Typically for two operators this leads to the condition of the commutativity of the operators, i.e., to the condition $[A_1, A_2] := A_1A_2 - A_2A_1 = 0$. In the sequel we investigate the necessity of this condition for the different kinds of splittings and for more than two sub-operators.

3.1. Sequential splitting

For the sequential splitting the following statements are true.

- The local splitting error of the sequential splitting with two sub-operators is zero if and only if A_1 and A_2 commute, which one can check directly.
- A necessary and sufficient condition for the sequential splitting with three sub-operators, A_1, A_2 and A_3, to have second order is

$$[A_2, A_1] + [A_3, A_1] + [A_3, A_2] = 0, \tag{3.7}$$

see [7]. Consequently, (3.7) is also a necessary condition for zero splitting error. Clearly, for (3.7) the pairwise commutativity, i.e. the condition

$$[A_1, A_2] = 0, \qquad [A_1, A_3] = 0 \quad \text{and} \quad [A_2, A_3] = 0, \tag{3.8}$$

is a sufficient condition. However, since (3.8) implies the relation $[A_3, A_2 + A_1] = [A_2 + A_1, A_3]$, therefore in this case for three operators we have

$$S_{\mathrm{seq}}(\tau) = \mathrm{e}^{A_3\tau}\mathrm{e}^{A_2\tau}\mathrm{e}^{A_1\tau} = \mathrm{e}^{(A_3+A_2+A_1)\tau} = S(\tau). \tag{3.9}$$

Hence, we have the following

Proposition 3.1. *If the three sub-operators pairwise commute, then local splitting error of the sequential splitting is zero.*

We remark that it is the rather strict sufficient condition (3.8) that one usually checks in air pollution models [2]. Note that it is not clear whether (3.8) is a necessary condition for zero local splitting error. We will now answer this question.

Consider the matrix

$$A = \begin{bmatrix} 4 & 2 \\ 0 & 3 \end{bmatrix} \tag{3.10}$$

and let us split it into the sum $A_1 + A_2 + A_3$ with

$$A_1 = A_3 = \begin{bmatrix} 3 & 1 \\ 0 & 2 \end{bmatrix} \quad \text{and} \quad A_2 = \begin{bmatrix} -2 & 0 \\ 0 & -1 \end{bmatrix}. \tag{3.11}$$

Then

$$\mathrm{e}^{tA} = \begin{bmatrix} \mathrm{e}^{4t} & 2\mathrm{e}^{3t}(\mathrm{e}^{t} - 1) \\ 0 & \mathrm{e}^{3t} \end{bmatrix}, \tag{3.12}$$

$$\mathrm{e}^{tA_1} = \mathrm{e}^{tA_3} = \begin{bmatrix} \mathrm{e}^{3t} & \mathrm{e}^{2t}(\mathrm{e}^{t} - 1) \\ 0 & \mathrm{e}^{2t} \end{bmatrix}, \quad \text{and} \quad \mathrm{e}^{tA_2} = \begin{bmatrix} \mathrm{e}^{-2t} & 0 \\ 0 & \mathrm{e}^{-t} \end{bmatrix}. \tag{3.13}$$

In this example A_1 and A_2 do not commute, since

$$[A_1, A_2] = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \tag{3.14}$$

but

$$\mathrm{e}^{\tau A_1}\mathrm{e}^{\tau A_2}\mathrm{e}^{\tau A_3} = \mathrm{e}^{\tau A}, \tag{3.15}$$

and so the sequential splitting is exact. Hence, the above example implies the following fact:

Proposition 3.2. *In the case of the sequential splitting with more than two sub-operators the commutation of each pair of sub-operators is not a necessary condition for zero local splitting error.*

3.2. Marchuk–Strang and SWS splittings

We note that for both the symmetric splittings and the SWS splitting the commutativity of the sub-operators is sufficient for zero splitting error.

However the necessity of the commutativity condition is unclear. If we consider example (3.10) with

$$A_1 = \begin{bmatrix} 6 & 2 \\ 0 & 4 \end{bmatrix} \quad \text{and} \quad A_2 = \begin{bmatrix} -2 & 0 \\ 0 & -1 \end{bmatrix}, \tag{3.16}$$

then $S_{\mathrm{MS}}(\tau) = S(\tau)$, i.e. the MS splitting is exact. However, $[A_1, A_2] \neq 0$. This implies the following

Proposition 3.3. *The commutation of the sub-operators in the MS splitting is not a necessary condition for zero local splitting error.*

For the SWS splitting let us consider the matrices

$$B = \begin{bmatrix} 5 & 1 \\ 0 & 3 \end{bmatrix}, \qquad B_1 = \begin{bmatrix} 3 & 1 \\ 0 & 2 \end{bmatrix}, \qquad B_2 = \begin{bmatrix} 2 & 0 \\ 0 & 1 \end{bmatrix}. \tag{3.17}$$

Then

$$\mathrm{e}^{tB} = \begin{bmatrix} \mathrm{e}^{5t} & 0.5\mathrm{e}^{5t} - 0.5\mathrm{e}^{3t} \\ 0 & \mathrm{e}^{3t} \end{bmatrix}, \tag{3.18}$$

$$\mathrm{e}^{tB_1} = \begin{bmatrix} \mathrm{e}^{3t} & \mathrm{e}^{3t} - \mathrm{e}^{2t} \\ 0 & \mathrm{e}^{2t} \end{bmatrix}, \quad \text{and} \quad \mathrm{e}^{tB_2} = \begin{bmatrix} \mathrm{e}^{2t} & 0 \\ 0 & \mathrm{e}^{t} \end{bmatrix}. \tag{3.19}$$

It is easy to check that $[B_1, B_2] \neq 0$, but $S_{\mathrm{SWS}}(\tau) = S(\tau)$. Consequently, we have

Proposition 3.4. *The commutation of the sub-operators in the SWS splitting is not a necessary condition for zero local splitting error.*

3.3. On the exact conditions of zero splitting error

As we mentioned in Section 3.1, the commutativity is a necessary and sufficient condition for the sequential splitting with two sub-operators to be exact. However, as we saw later on, for the MS and SWS splittings, just as for the sequential splitting with more than two sub-operators, the pairwise commutativity is only sufficient, but not necessary for the vanishing of the splitting error. New necessary conditions, similar to that under (3.7), can be created by eliminating the coefficients of higher order terms in the Taylor series expansion of the local splitting error. However, the strict conditions imposed on transport-chemistry problems, like (3.8), may not be necessary.

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